

# Electronic Localization Properties of a Double Strand of DNA: A Simple Model with Long-Range Correlated Hopping Disorder

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## Abstract

Localization property in the disordered few-chain DNA systems with a long-range correlation is numerically investigated. We apply the chain system with the correlated disorder in the interchain and/or intrachain hoppings to the simple model of a double strand of DNA. Numerical results for the density of states and the Lyapunov exponent of the wave function in the two- or three-chain models are given. It is found that the correlation effect enhances the localization length (the inverse least nonnegative Lyapunov exponent) around the band center.

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## I. INTRODUCTION

Localization phenomena in the one-dimensional disordered system have been extensively studied [1]. It is well known that almost all the eigenstates are exponentially localized and the system has a pure point energy spectrum under the presence of any disorder [2]. Recently, the effect of the long-range correlated disorder in the potential field on the localization has been reported by some groups [3, 4, 5, 6, 7]. The appearance of the Anderson-like metal-insulator transition is suggested in the strongly correlated non-stationary regime of the sequence [4]. As one of the realistic situation, it has been found that the base (nucleotide) sequence of the various genes has a strong correlation characterized by the power spectrum  $S(f) \sim f^{-\alpha}$  ( $0.2 < \alpha < 0.8$ ) [5, 8, 9, 10, 11, 12, 13].

Moreover, the recent development of the nanoscale fabrication let us expect the utilization of the DNA wire as a molecular device [14, 15] and the realization of DNA computing [16, 17]. Actually, the development enables us to measure the direct DNA transport phenomena [15, 18, 19, 20]. Recently, Porth *et al.* measured the nonequilibrium current-voltage ( $I - V$ ) characteristics in the poly(G)-poly(C) DNA molecule attached to platinum lead at room temperature [18]. Cuniberti *et al.* explained the semiconducting behavior by considering the base-pair stack coupled to the sugar-phosphate(SP) backbone pair [21]. Iguchi also derived the semiconductivity and the band gap by using the ladder chain model of the double strand of DNA [20, 22, 23]. In the both models, apparently, the existence of the SP backbone chain play an important role in the band structure due to the gap opening by the hybridization of the energy levels.

On the other hand, recently Tran et al measured the conductivity along the lambda phage DNA ( $\lambda$ -DNA) double helix at microwave frequencies using the lyophilized DNA in and also without a buffer [19]. The conductivity is strongly temperature dependent around room temperature with a crossover to a weakly temperature dependent conductivity at low temperatures. Yu and Song showed that the observed temperature dependent conductivity in the DNA can be consistently modeled, without invoking the additional ionic conduction mechanisms, by considering that electrons may use the variable range hopping for conduction and that electron localization is enhanced by strong thermal structural fluctuations in DNA [24]. Then the DNA double helix is viewed as a one-dimensional Anderson system.

As observed in the power spectrum, the mutual information analysis and the Zipf analysis

of the DNA base sequence such as the human chromosome 22, the long-range structural correlation exists in the total sequence as well as the short-range periodicity [10, 11, 12, 13]. The transport property though DNA are still controversial mainly due to the complexity of the experimental environment and the molecule itself. Although the theoretical explanations for the phenomena have been tried by some standard pictures used in the solid state physics such as polarons, solitons, electrons or holes [14, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37], the situation is still far from unifying the theoretical scheme.

In the present paper we investigate the correlation effect on the localization property of the one-electronic states in the disordered, two-chain (ladder) [38] and three-chain models with a long-range structural correlation as a simple model for the electronic property in the DNA. The tight-binding model for the few-chain systems have the off-diagonal randomness as the interchain hopping integral and/or the intrachain ones. We present some numerical results for the density of states (DOS) and the Lyapunov exponents of the wave function. In particular, it is found that the correlation of the sequence enhances the localization length defined by using the least nonnegative Lyapunov exponent. Regardless of the parameter tuning for the numerical calculation, we would like to mainly focus on (1)suggesting the model and (2)giving the preliminary numerical results for the correlation effect on the localization in the model.

Outline of the present paper is as follows. In the next section we introduce the models for DNA with a long-range correlation. In the Sect.3 we give the results for the density of states. The numerical results for the Lyapunov exponent and the localization length in the systems are given in Sect.4. The last section devotes for summary and discussion.

## II. MODEL

We simplify and model the double strand of DNA by some assumptions. DNA double helix structure is constructed by the coupled two single strand of DNA. First, we ignore the twist of DNA as well as the complicated topology. (See Fig.1.) In addition to the simplification, we consider only the  $\pi$ -electrons with the highest occupied molecular orbit (HOMO) states in the backbones and the base-pairs of the system. We also ignore the interaction between the electrons and restrict ourselves to the zero-temperature property.

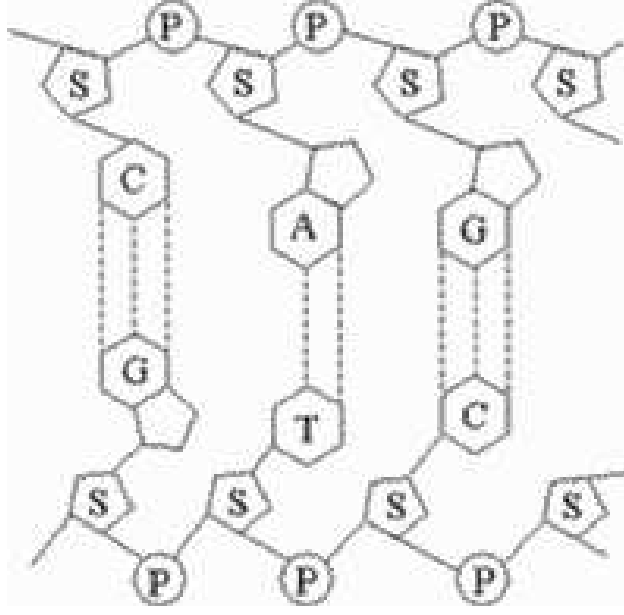


FIG. 1: The schematic structure of a double strand of DNA.

### A. Two-chain model

Following the basic assumptions, consider the one-electron system described by the tightly binding Hamiltonian  $\hat{H}$  consisting of the two chains. This model was first given by Iguchi [22, 23] as a model for considering the electronic properties of a double strand of DNA.

$$\hat{H} = H_A + H_B + H_{AB}, \quad (1)$$

$$H_k = \sum_n \{k_{n,n}|k:n\rangle\langle k:n| - (k_{n+1,n}|k:n+1\rangle\langle k:n| + h.c.)\}, \quad (2)$$

$$H_{AB} = -\sum_n V_n(|A:n\rangle\langle B:n| + |B:n\rangle\langle A:n|), \quad (3)$$

where the  $\{|A:n\rangle, |B:n\rangle\}$  denotes an orthonormalized set and  $A_{n+1,n}$  ( $B_{n+1,n}$ ) means the hopping integral between the  $n$ th and  $(n+1)$ th sites and  $A_{n,n}$  ( $B_{n,n}$ ) the on-site energy at site  $n$  in chain  $A$  ( $B$ ), and  $V_n$  is the hopping integral from chain  $A(B)$  to chain  $B(A)$  at site  $n$ , respectively. The Schrödinger equation  $\hat{H}|\Psi\rangle = E|\Psi\rangle$  becomes,

$$A_{n+1,n}\phi_{n+1}^A + A_{n,n-1}\phi_{n-1}^A + A_{n,n}\phi_n^A + V_n\phi_n^B = E\phi_n^A,$$

$$B_{n+1,n}\phi_{n+1}^B + B_{n,n-1}\phi_{n-1}^B + B_{n,n}\phi_n^B + V_n\phi_n^A = E\phi_n^B,$$

where  $\phi_n^A \equiv \langle A : n | \Psi \rangle$  and  $\phi_n^B \equiv \langle B : n | \Psi \rangle$ . Furthermore it can be rewritten in the matrix form,

$$\begin{pmatrix} \phi_{n+1}^A \\ \phi_{n+1}^B \\ \phi_n^A \\ \phi_n^B \end{pmatrix} = \begin{pmatrix} \frac{E-A_{nn}}{A_{n+1n}} & -\frac{V_n}{B_{n+1n}} & -\frac{A_{n-1n}}{A_{n+1n}} & 0 \\ -\frac{V_n}{B_{n+1n}} & \frac{E-B_{nn}}{B_{n+1n}} & 0 & -\frac{B_{n-1n}}{B_{n+1n}} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \phi_n^A \\ \phi_n^B \\ \phi_{n-1}^A \\ \phi_{n-1}^B \end{pmatrix} \equiv T(n) \begin{pmatrix} \phi_n^A \\ \phi_n^B \\ \phi_{n-1}^A \\ \phi_{n-1}^B \end{pmatrix}. \quad (4)$$

Generally speaking, we would like to investigate the asymptotic behavior ( $n \rightarrow \infty$ ) of the products of the matrices  $M_n = \Pi_k^n T(k)$ . According to the parameter sets given by Iguchi [23], we set  $A_{n+1,n} = B_{n+1,n} = a(=b)$  at odd (even) site  $n$ , respectively and  $V_n = 0$  at even sites (phosphate sites) for simplicity. The chain  $A$  and  $B$  are constructed by the repetition of the sugar-phosphate sites, and the inter-chain hopping  $V_n$  at the sugar sites come from the nucleotide base-pairs, i.e.,  $A - T$  or  $G - C$  pairs. (See Fig.2(a).)

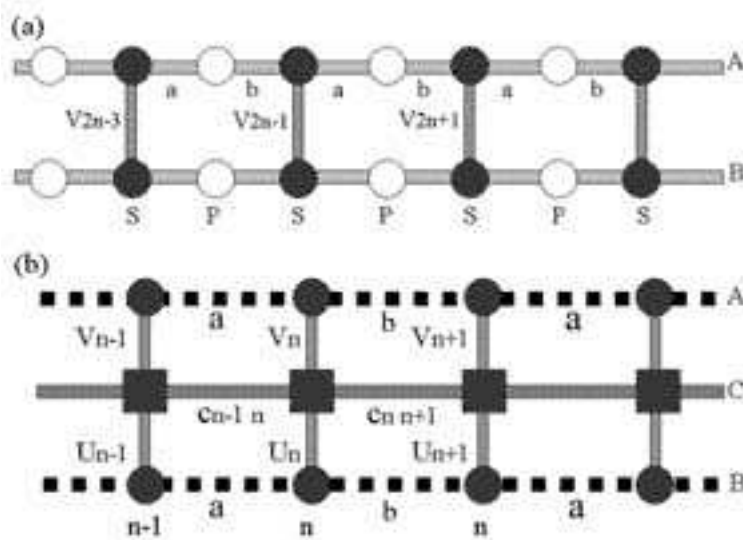


FIG. 2: Models of the double strand of DNA. (a) the two-chain model, (b) the three-chain model.

## B. Three-chain model

When we pay attention to the overlap integral between the nucleotide base-pairs, the two-chain model can be easily extended to the three-chain one described by following Hamil-

tonian. (See Fig.2(b).)

$$\hat{H} = H_A + H_B + H_C + H_{AC} + H_{BC}, \quad (5)$$

$$H_{AC} + H_{BC} = - \sum_n (V_n |A : n\rangle \langle C : n| + U_n |B : n\rangle \langle C : n| + h.c.), \quad (6)$$

where the  $\{|A : n\rangle, |C : n\rangle, |B : n\rangle\}$  denotes an orthonormalized set and  $C_{n+1,n}$  means the hopping integral between the  $n$ th and  $(n+1)$ th sites and  $C_{n,n}$  the on-site energy at site  $n$  in chain  $C$ , and  $V_n$  and  $U_n$  are the hopping integral between the chains. The Schrödinger equation  $\hat{H}|\Psi\rangle = E|\Psi\rangle$  becomes,

$$\begin{aligned} A_{n+1,n}\phi_{n+1}^A + A_{n,n-1}\phi_{n-1}^A + A_{n,n}\phi_n^A + V_n\phi_n^C &= E\phi_n^A, \\ C_{n+1,n}\phi_{n+1}^C + C_{n,n-1}\phi_{n-1}^C + C_{n,n}\phi_n^C + V_n\phi_n^A + U_n\phi_n^B &= E\phi_n^C, \\ B_{n+1,n}\phi_{n+1}^B + B_{n,n-1}\phi_{n-1}^B + B_{n,n}\phi_n^B + U_n\phi_n^C &= E\phi_n^B, \end{aligned}$$

where  $\phi_n^C \equiv \langle C : n | \Psi \rangle$ . It can be rewritten in the matrix form,

$$\begin{pmatrix} \Phi_{n+1} \\ \Phi_n \end{pmatrix} = T(n) \begin{pmatrix} \Phi_n \\ \Phi_{n-1} \end{pmatrix}, T(n) = \begin{pmatrix} H_d & H_o \\ I & O \end{pmatrix}. \quad (7)$$

where  $\Phi_n = (\phi_n^A, \phi_n^C, \phi_n^B)^t$  and  $I$  and  $O$  denote the three-dimensional unit and zero matrices, respectively. The matrices  $H_d$  and  $H_o$  are given as follows:

$$H_d = \begin{pmatrix} \frac{E-A_{nn}}{A_{n+1n}} & -\frac{V_n}{A_{n+1n}} & 0 \\ -\frac{V_n}{C_{n+1n}} & \frac{E-C_{nn}}{C_{n+1n}} & -\frac{U_n}{C_{n+1n}} \\ 0 & -\frac{U_n}{B_{n+1n}} & \frac{E-B_{nn}}{B_{n+1n}} \end{pmatrix}, H_o = \begin{pmatrix} -\frac{A_{n-1n}}{A_{n+1n}} & 0 & 0 \\ 0 & -\frac{C_{n-1n}}{C_{n+1n}} & 0 \\ 0 & 0 & -\frac{B_{n-1n}}{B_{n+1n}} \end{pmatrix}. \quad (8)$$

In this paper we set  $A_{n+1,n} = B_{n+1,n} = a(=b)$  at odd(even) site  $n$ , and  $V_n = U_n$ . (See Fig.2(b).) In addition, in the numerical calculation we set the on-site energy as  $A_{nn} = B_{nn} = C_{nn} = 0$  for simplicity. The sequence  $\{C_{nn+1}\}$  can be also generated by corresponding to the base-pairs sequence. The localization properties in the simple few-chain models with the on-site disorder have been extensively investigated [39].

### C. The correlated sequence

The correlated binary sequence  $\{V_n\}$  and/or  $\{C_{nn+1}\}$  of the hopping integrals can be generated by the modified Bernoulli map [3, 40, 41, 42].

$$X_{n+1} = \begin{cases} X_n + 2^{B-1}X_n^B & (X_n \in I_0) \\ X_n - 2^{B-1}(1 - X_n)^B & (X_n \in I_1), \end{cases} \quad (9)$$

where  $I_0 = [0, 1/2)$ ,  $I_1 = [1/2, 1)$ .  $B$  is a bifurcation parameter which controls the correlation of the sequence.

In the ladder model we use the symbolized sequence  $\{V_n\}$  by the following rule as the interchain hopping integral at odd sites  $n$ :

$$V_n = \begin{cases} W_{AT} = W_{TA} & (X_n \in I_0) \\ W_{GC} = W_{CG} & (X_n \in I_1). \end{cases} \quad (10)$$

In the numerical calculation, we use  $W_{GC} = W_{AT}/2$  for simplicity. Then the artificial binary sequence can be roughly regarded as the base-pair sequence as observed in the  $\lambda$ -DNA or the human chromosome 22. The correlation function  $C(n)(\equiv \langle V_{n_0} V_{n_0+n} \rangle)$  ( $n_0 = 1$ ,  $n$  is even) decays by the inverse power-law depending on the value  $B$  as  $C(n) \sim n^{-\frac{2-B}{B-1}}$  for large  $n$  ( $3/2 < B < 2$ ). The power spectrum becomes  $S(f) \sim f^{-\frac{2B-3}{B-1}}$  for small  $f$ . We focus on the Gaussian ( $1 < B < 3/2$ ) and the non-Gaussian stationary region  $2/3 \leq B < 2$ , corresponding to the DNA base-pairs sequence ( $0.2 < \alpha < 0.8$ ).

In the three-chain model we assume that the phosphate sites are renormalized in the hopping integral between the sugar sites for simplicity. The interchain hopping integrals  $V_n = U_n$  can be generated by the same way to the two-chain model for every site  $n$ . Furthermore, we use the successive sequence  $\{X_n, X_{n+1}\}$  when we make the correlated binary sequence  $\{C_{nn+1}\}$  as the hopping integral of the middle (nucleotide) chain as follows:

$$C_{nn+1} = \begin{cases} W_{AT-AT} & (X_n \in I_0, X_{n+1} \in I_0) \\ W_{AT-GC} & (X_n \in I_0, X_{n+1} \in I_1) \\ W_{GC-AT} & (X_n \in I_1, X_{n+1} \in I_0) \\ W_{GC-GC} & (X_n \in I_1, X_{n+1} \in I_1). \end{cases} \quad (11)$$

In the numerical calculation we assume the following rules for simplicity.

$$\begin{cases} W_{GC-GC} = W_{AT-AT}/2 \\ W_{AT-GC} = (W_{AT-AT} + W_{GC-GC})/2 \\ W_{GC-AT} = W_{AT-GC}. \end{cases} \quad (12)$$

As a result, the parameters are  $W_{AT}$  and  $W_{AT-AT}$ .

### III. DENSITY OF STATES AND LYAPUNOV EXPONENTS

In this section, we show the DOS and the Lyapunov exponents for the periodic and disordered two-chain model in order to give some notations and to confirm the numerical reliability.

Let us consider the periodic case to confirm the gap opening mechanism due to hybridization by the interchain coupling. Figure 3 shows the DOS for various periodic cases. As seen in the Fig.3(b) the energy spectrum consists of four bands when  $W_{AT} = W_{GC}$  and  $A_{nn} = B_{nn} = 0$ . The band gap  $E_g(v)$  at the center is given by  $E_g(v) = \sqrt{(E_g^2 + v^2)} - v$ , where  $E_g \equiv 2(a - b)$  means the band gap for the single strand of DNA. The other band gap  $\Delta_g(v) = v + \frac{1}{2}[\sqrt{(E_g^2 + v^2)} + \sqrt{4(a + b)^2 + v^2}]$  appears in between the lowest and the lower middle bands where  $v > 2ab/\sqrt{(a^2 + b^2)}$ . Iguchi showed the semiconductivity of the double strand of DNA based on the band structure [23, 26]. The energy spectrum in the case  $a = b$  is given in Fig.3(a). The band gap at the center disappears. Furthermore, the energy band for case  $W_{AT} \neq W_{GC}$  ( $W_{GC} = W_{AT}/2$ ) is shown in Fig.3(c). Each band splits and the total spectrum consists of eight bands.

Figure 4 shows the DOS as a function of the energy for the binary disordered system. The sequence of the interchain hopping takes an alternative value  $W_{GC}$  or  $W_{AT}$ . It is found that some gaps observed in the periodic cases close due to the disorder corresponding to the base-pairs sequence.

It is noted that in the bipartite lattice with an even number of sites the energy spectrum is striking symmetric around  $E = 0$  [43, 44, 45, 46, 47, 48]. In this case, related to the chiral universality class, the  $E = 0$  states are non-localized in any dimension. However, the states with the Dyson singularity [49] at the center disappear when the randomness is introduced in the on-site energy at the backbone chains. We comment the point in the next section again.

We give a preliminary numerical result of the energy dependence of the Lyapunov exponents. The definition is given by,

$$\gamma_i = \lim_{n \rightarrow \infty} \frac{1}{2n} \log \sigma_i(M_n^\dagger M_n), \quad (13)$$

where  $\sigma_i(\dots)$  denotes the  $i$ th eigenvalue [41]. As the transfer matrix  $T(n)$  is symplectic, the eigenvalues of the  $M_n^\dagger M_n$  have the reciprocal symmetry around the unity as



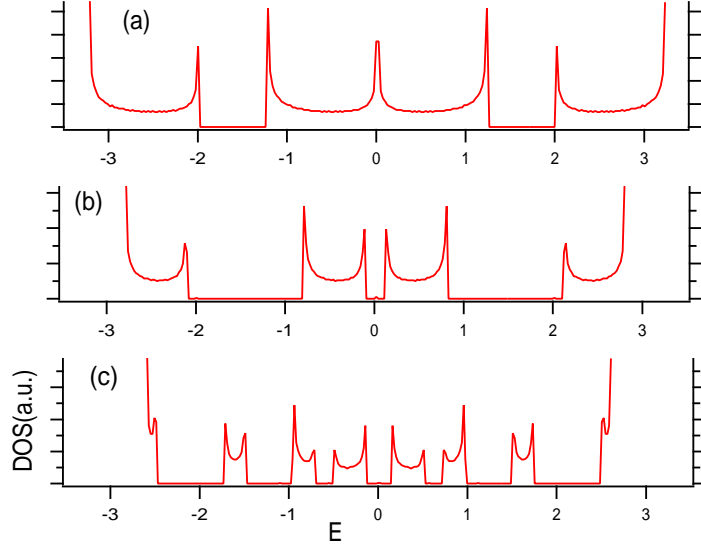


FIG. 3: DOS as a function of energy for the periodic cases in the two-chain model. (a)  $W_{AT} = W_{GC} = 2.0, a = 1.0, b = 1.0$ . (b)  $W_{AT} = W_{GC} = 2.0, a = 1.0, b = 0.5$ . (c)  $W_{AT} = 2.0, W_{GC} = 1.0, a = 1.0, b = 1.0$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ .

$e^{\gamma_1}, \dots, e^{\gamma_d}, e^{-\gamma_d}, \dots, e^{-\gamma_1}$ , where  $\gamma_1 \geq \gamma_2 \geq \dots \gamma_d \geq 0$ . The  $d$  denotes the number of channels, i.e.  $d = 2$  in the two-chain model and  $d = 3$  in the three-chain model.

Figure 5 shows all of the Lyapunov exponents  $\gamma_i (i = 1, 2, 3, 4)$  as a function of the energy to confirm the reciprocal symmetry. The energy regions where two exponents are positive ( $\gamma_1 > \gamma_2 > 0$ ) correspond to the energy gap in Fig.3 except for the vicinity of the singular point  $E = 0$ . The zero Lyapunov exponent corresponds to the brunch cut in the analyticity of the energy spectrum.

The Lyapunov exponents are related to the DOS  $\rho(E)$  as an analogue of the Thouless relation as [50, 51],

$$\sum_i^d \gamma_i(E) \sim \int \ln |E - E'| \rho(E') dE'. \quad (14)$$

Note that the Thouless relation ( $d = 1$ ) is true only for the positive Lyapunov exponents. One can see that the singularity of the largest Lyapunov exponent is strongly related to the singularity of the DOS.

Furthermore, it is found that for the thermodynamic limit the largest channel-dependent localization length  $\xi_d = 1/\gamma_d$  determines the exponential decay of the Landauer conductance

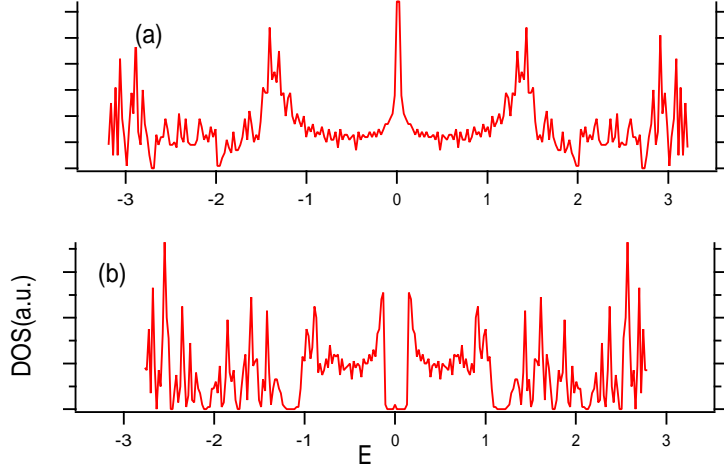


FIG. 4: DOS as a function of energy for the binary disordered cases in the two-chain model. (a)  $W_{AT} = 2.0, W_{GC} = 1.0, a = 1.0, b = 1.0$ . (b)  $W_{AT} = 2.0, W_{GC} = 1.0, a = 1.0, b = 0.5$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ .

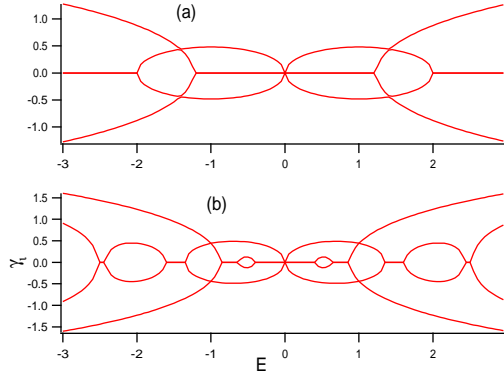


FIG. 5: Lyapunov exponents as a function of energy for the periodic cases in the two-chain model. (a)  $W_{AT} = W_{GC} = 2.0, a = 1.0, b = 1.0$ . (b)  $W_{AT} = 2.0, W_{GC} = 1.0, a = 1.0, b = 1.0$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ .

$g$  which is in units of  $e^2/h$  at zero temperature and serves as the localization length of the total system of the coupled chains [52, 53].

$$g(m) = 2 \sum_{i=1}^d \frac{1}{\cosh \frac{2m}{\xi_i(m)} - 1} \sim \exp\left(-\frac{2m}{\xi_d(m)}\right). \quad (15)$$

Recently, electron transport for the molecular wire between two metallic electrodes has been also investigated by several techniques [54, 55, 56, 57].

#### IV. CORRELATION EFFECTS

In this section, we consider the correlation effect on the localization property of the disordered case by using the modified Bernoulli model. Figure 6 shows some eigenstates for the correlated case,  $B = 1.8$ . Apparently the eigenstates are exponentially localized. In particular, the energy dependence of the Lyapunov exponents and the localization length are investigated in order to characterize the localization. We used a large sample with the system size  $N = 10^6$  for the numerical calculation.

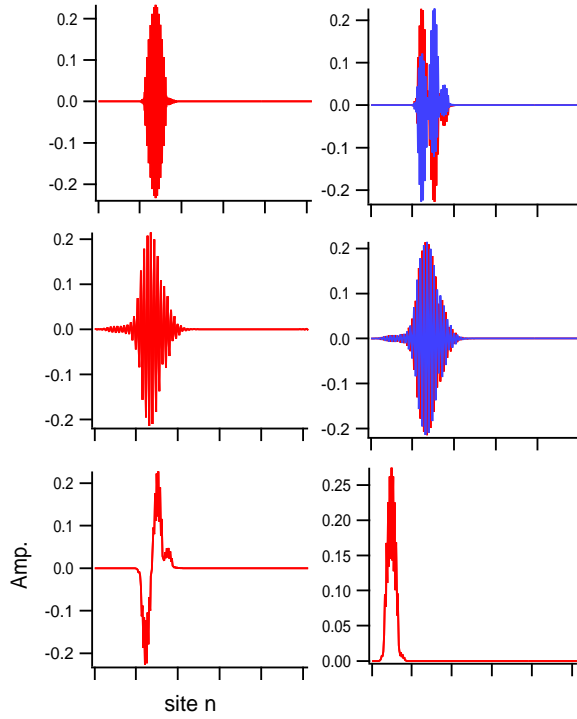


FIG. 6: Some eigenfunctions for the binary correlated disordered cases  $B = 1.8$  in the two-chain model ( $N = 256$ ). The amplitude of the wave function for A and B chains are over-written.  $W_{AT} = 2.0$ ,  $W_{GC} = 1.0$ ,  $a = 1.0$ ,  $b = 0.5$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ .

##### A. Two-chain model

First, we show the expectable results by a simple analytical calculation. We can write the Schrödinger equation in the following matrix form when the hopping integral and the

on-site energy of the backbone chains are the same values ( $a = b, A_{nn} = B_{nn}$ ),

$$\begin{pmatrix} \phi_{n+1}^A + \phi_{n-1}^A \\ \phi_{n+1}^B + \phi_{n-1}^B \end{pmatrix} = \frac{1}{a} \begin{pmatrix} E - A_{nn} & -V_n \\ -V_n & E - B_{nn} \end{pmatrix} \begin{pmatrix} \phi_n^A \\ \phi_n^B \end{pmatrix}.$$

It is easily seen that the equations can be decoupled to the one-dimensional Anderson model with diagonal randomness by the unitary transform  $U$  as follows;

$$\begin{pmatrix} \psi_n^A \\ \psi_n^B \end{pmatrix} = U \begin{pmatrix} \phi_n^A \\ \phi_n^B \end{pmatrix}, U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (16)$$

$$\begin{pmatrix} \psi_{n+1}^A + \psi_{n-1}^A \\ \psi_{n+1}^B + \psi_{n-1}^B \end{pmatrix} = \frac{1}{a} \begin{pmatrix} E - V_n - \mu_n & \nu_n \\ \nu_n & E + V_n - \mu_n \end{pmatrix} \begin{pmatrix} \psi_n^A \\ \psi_n^B \end{pmatrix}, \quad (17)$$

where

$$\mu_n = \frac{1}{2}(A_{nn} + B_{nn}), \nu_n = \frac{1}{2}(A_{nn} - B_{nn}). \quad (18)$$

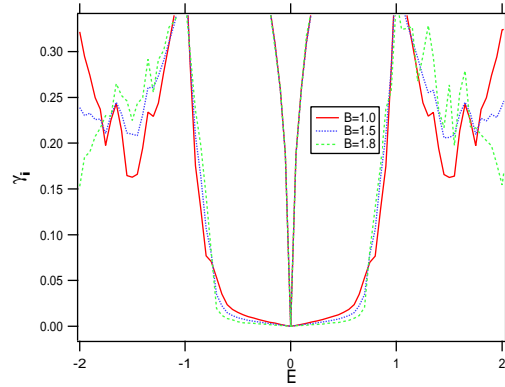


FIG. 7: Lyapunov exponents  $\gamma_i (i = 1, 2)$  as a function of energy in the correlated two-chain model. The parameters  $W_{AT} = 2.0, a = 1.0, b = 1.0$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ . The number of the matrix product is  $N = 10^6$ .

In our case,  $\mu_n = A_{nn}, \nu_n = 0$ . Accordingly, the behavior of the Lyapunov exponents are essentially the same to that in the one-dimensional system with the sublattice diagonal disorder. After all the  $V_n$  is non-zero only if  $n$  is odd, i.e.  $V_{2n-1}$  is random and  $V_{2n} = 0$ . Sometime the model is called the "periodic random alloy" or the "dilute Anderson model" [43, 46]. Although in our case the energy at the deterministic even sites are zero, the case

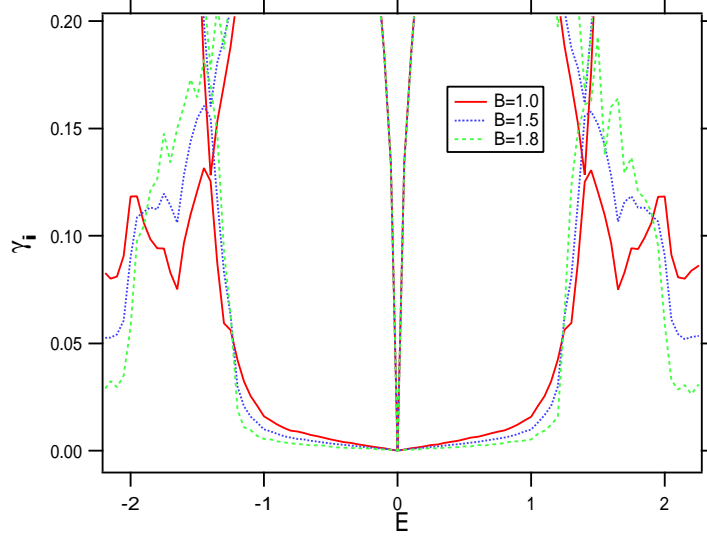


FIG. 8: Lyapunov exponents  $\gamma_i (i = 1, 2)$  as a function of energy in the correlated two-chain model. The parameters  $W_{AT} = 2.0, a = 1.0, b = 0.5$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ . The number of the matrix product is  $N = 10^6$ .

where the deterministic sites are non-zero but constant is trivially obtained by shifting the energy. The extended state at  $E = 0$  appears in the one-dimensional periodic random binary alloys due to a resonance [46, 58]. It is demonstrated that the occurrence of the extended states in the vicinity of the site energy of the deterministic part, i.e.  $E = 0$  in our case. The delocalization can be understood in terms of the long-range correlation due to the perfect periodicity in the deterministic sites.

In addition, we introduce another long-range correlation due to the base-pair sequence on the odd sites  $V_{2n-1}$ . Figures 7 and 8 show the energy dependence of the Lyapunov exponents ( $\gamma_1$  and  $\gamma_2$ ) in some correlated cases ( $B = 1.0, 1.5, 1.8$ ). It found that the correlation enhances the localization length  $\xi (\equiv \gamma_2^{-1})$  around  $|E| < 1$ , although the largest Lyapunov exponent  $\gamma_1$  is almost remained.

In Fig.9(a) the localization length  $\xi_d = 1/\gamma_d$  defined by the least nonnegative Lyapunov exponent is shown. The electronic states whose energy is close to the resonance turn out to be extended in the sense that the localization length is the same order or larger than the system size. Accordingly the correlation effect is not so strong on the global feature in the energy dependence of the density of states, particularly the correlation enhances the localization length in the energy regime  $|E| < 1$ .

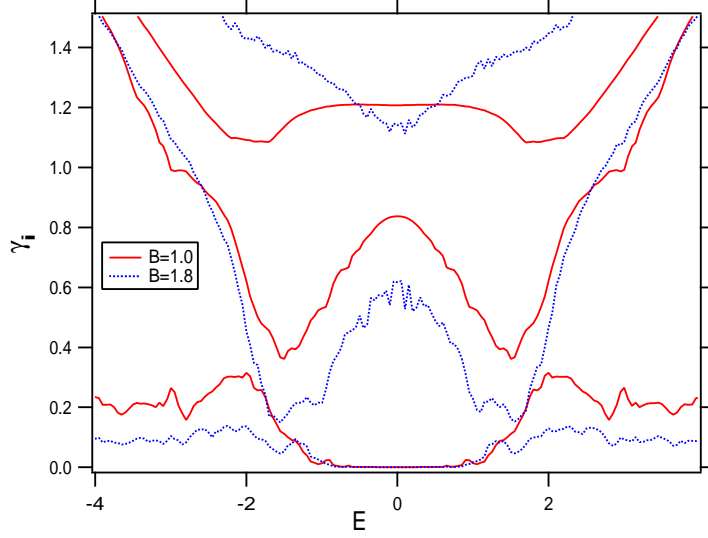


FIG. 9: Localization length  $\xi(=1/\gamma_2)$  as a function of energy in the correlated (a)two-chain model and (b)three-chain model. The parameters  $W_{AT} = 2.0, W_{AT-AT} = 1.0, a = 1.0, b = 0.5$ . The on-site energy is set at  $A_{nn} = B_{nn} = 0$ . The number of the matrix product is  $N = 10^6$ .

### B. Three-chain model

In this subsection, we confirm the numerical results for the three-chain model when compared to that in the two-chain model. It must be noted that if we take into account of a  $\pi - \pi$  interaction between the stacked base pairs, the model system becomes three chains model. (See Fig.2(b).)

As has been done in the two-chain case we can rewrite the Schrödinger equation in the matrix form as follows,

$$\begin{pmatrix} \phi_{n+1}^A + \phi_{n-1}^A \\ \phi_{n+1}^C + \phi_{n-1}^C \\ \phi_{n+1}^B + \phi_{n-1}^B \end{pmatrix} = \begin{pmatrix} E - A_{nn} & -V_n & 0 \\ -\frac{V_n}{t_c} & \frac{E - C_{nn}}{t_c} & \frac{U_n}{t_c} \\ 0 & U_n & E - B_{nn} \end{pmatrix} \begin{pmatrix} \phi_n^A \\ \phi_n^C \\ \phi_n^B \end{pmatrix} \equiv R \begin{pmatrix} \phi_n^A \\ \phi_n^C \\ \phi_n^B \end{pmatrix}. \quad (19)$$

We set  $a = b = 1, C_{nn+1} = t_c$  for simplicity. It should be noted that the matrix  $R$  can not be diagonalized by any unitary transform because the matrix is not a normal matrix,  $R^t R \neq R R^t$ , when  $t_c \neq 1$  (Toeplitz theorem). Accordingly the simple expectation in the previous subsection is not suitable for the three-chain model.

Figures 10 and 11 show the energy dependence of the Lyapunov exponents in the three chain cases. We can observe that all the Lyapunov exponents  $\gamma_i (i \leq d)$  are changed by the

correlation. The least nonnegative Lyapunov exponent  $\gamma_3$  is diminished by the correlation. The localization length are shown in Fig.9(b). We can see that the localization length diverges at the band center  $E = 0$ .

Generally speaking, in the quasi-one-dimensional chain with the hopping disorder the singularity of DOS, the localization length and the conductance at the band center depend on the parity, bipartiteness and the boundary condition [46, 48]. As the discussion about the details is out of scope of this paper, we give the simple comment. Note that the parity effects appear in the odd number chain with the hopping randomness. In the odd number chain with a hopping randomness, only one mode at  $E = 0$  is remained as the extended state, i.e.  $\gamma_d = 0$ , and the other exponents are positive,  $\gamma_{d-1} > \dots > \gamma_1 > 0$ . The behavior is seen in Fig.10 and 11. Then, the non-localized states with  $\gamma = 0$  determine the conductance. Although we ignored the bipartite structure in the three-chain model for simplicity, if we introduce the bipartiteness in the intrachain hopping integral  $V_n (= U_n)$  the other delocalized state due to the chiral symmetry appears at  $E = 0$  as seen in the ladder model.

Here, we stress again that in the more realistic model of DNA the parity effects and the chiral symmetry are broken down by the on-site energy fluctuation. Indeed, Fig.12(a) shows the energy dependence of the Lyapunov exponents in the system which the on-site energy  $A_{nn} (= B_{nn})$  in the side chains is also randomly generated as well as the hopping disorder in Fig.11. In this case we can confirm that the least nonnegative Lyapunov exponent,  $\gamma_3$ , is positive. It is found that the extended state at  $E = 0$  disappears and the localization length becomes finite. (See Fig.12(b).) As a result, the localization properties can be changed by the introduction of the correlation and the fluctuation of the sequence even in scope of our models.

## V. SUMMARY AND DISCUSSION

We numerically investigated the correlation effect on the localization property of the one-electronic states in the disordered two-chain (ladder) and three-chain models with the long-range structural correlation as the simple models for electronic property in the double strand of DNA. The results are summarized as follows.

(1) We gave the tight-binding models for the few-chain systems with the off-diagonal randomness as the interchain and/or the intrachain hopping integrals.

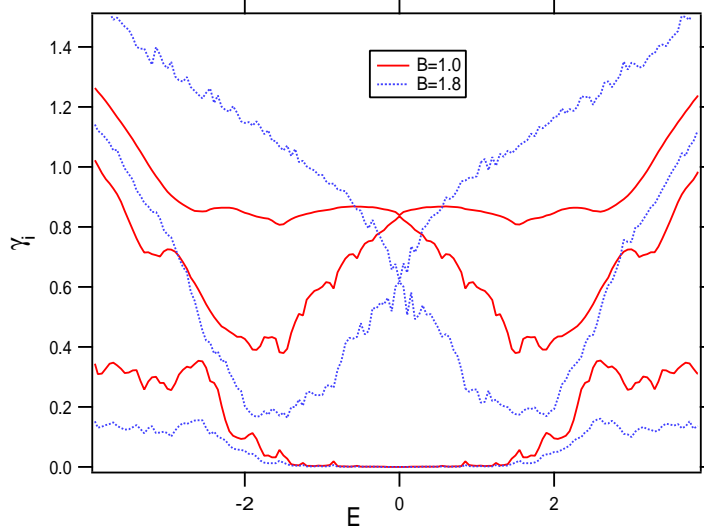


FIG. 10: Lyapunov exponents  $\gamma_i$  ( $i = 1, 2, 3$ ) as a function of energy in the correlated three-chain model. The parameters  $W_{AT} = 2.0$ ,  $W_{AT-AT} = 1.0$ ,  $a = 1.0$ ,  $b = 1.0$ . The on-site energy is set at  $A_{nn} = B_{nn} = C_{nn} = 0$ .

(2) A simple interpretation for the results obtained in the two-chain model was given by means of the unitary transform.

(3) The correlation enhances the localization length ( $\gamma_2^{-1}$ ) around  $|E| < 1$ , although the  $\gamma_1$  is almost remained, in the two-chain model.

(4) In the three-chain model, all the Lyapunov exponents are changed by the correlation effect, particularly, the least nonnegative exponent  $\gamma_3$  is diminished by the long-range correlation.

(5) The divergence of the localization length around the  $E = 0$  disappears by the introduction of the fluctuation of the on-site energy.

The details of the energy dependence, the correlation dependence and the potential strength dependence on the DOS and the Lyapunov exponents, will be given elsewhere [59].

Although we concentrated on the localization property of the correlated system for the double strand of DNA by using simple values for the parameters, the more realistic Hamiltonian matrix elements are obtained from the oligomer calculation using the extended Hückel theory with the Clementi's parametrization [26, 60, 61, 62].

In the experiment of the conductance property of the DNA both the temperature de-



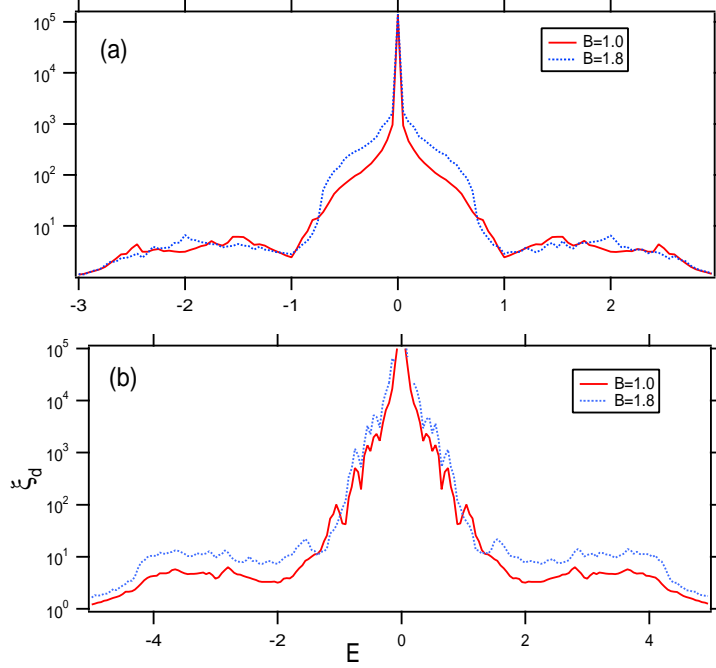


FIG. 11: Lyapunov exponents  $\gamma_i (i = 1, 2, 3)$  as a function of energy in the correlated three-chain model. The parameters  $W_{AT} = 2.0, W_{AT-AT} = 1.0, a = 1.0, b = 0.5$ . The on-site energy is set at  $A_{nn} = B_{nn} = C_{nn} = 0$ .

pendence and the temperature effect are important. Finite temperature can also reduce the effective system size and leads to the changes in the transport property. Moreover, the effects of the stacking energy and of temperature can be considered by introducing the fluctuation in the hopping energy such as the Su-Schrieffer-Heeger model for polyacetylene [63]. It is interesting to investigate the quantum diffusion in order to reveal the conducting properties of electrons, polarons and solitons in the fluctuating ladder models [59]. In the present model, although we used the binary correlated sequence, the four letter version (A,T,G,C) is also interesting [64]. An extension for the four letter version with a long-range correlated hopping disorder has been constructed [59].

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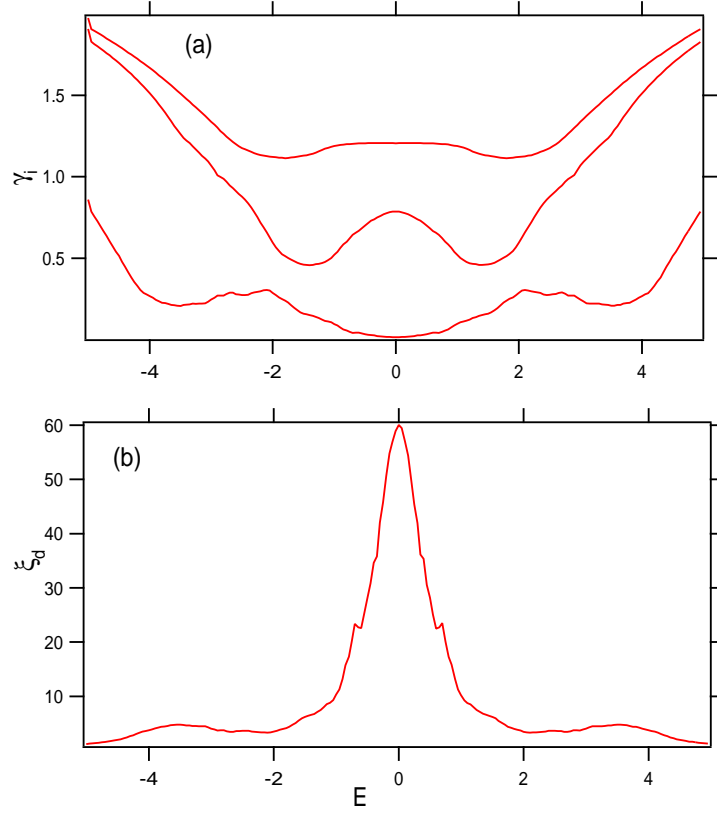


FIG. 12: (a) Lyapunov exponents  $\gamma_i (i = 1, 2, 3)$  as a function of energy in the disordered three-chain model ( $B = 1.0$ ). (b) The localization length defined by  $\xi_d \equiv 1/\gamma_3$ . The parameters  $W_{AT} = 2.0, W_{AT-AT} = 1.0, a = 1.0, b = 0.5$  and  $C_{nn} = 0$ . The on-site energy of the side chains,  $A_{nn}(= B_{nn})$ , is randomly generated.

study.

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- [1] See, for example, L.M. Lifshiz, S.A. Gredeskul and L.A. Pastur, *Introduction to the theory of Disordered Systems*, (Wiley, New York, 1988).
  - [2] K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77(1973).
  - [3] H. Yamada, M. Goda and Y. Aizawa, J. Phys.:Condens. Matter **3**, 10043(1991).
  - [4] F.A.B.F. de Moura and M.L. Lyra, Phys. Rev. Lett. **81**, 3735(1998).
  - [5] P. Carpena, P.B. Galvan, P.Ch. Ivanov and H.E. Stanley, Nature **418**, 955(2002); *ibid*, **84**, 764(2003).
  - [6] H. Yamada, J. Phys. Soc. Jpn. Suppl. A **72**, 123(2003).

- [7] H. Yamada, Phys. Rev. B, in press.
- [8] R.F. Voss, Phys. Rev. Lett. **68**, 3805(1992).
- [9] *DNA and Protein Sequence Analysis: A Practical Approach*, (IRL press, 1997), Ed. by M.J. Bishop and C.J. Rawlings.
- [10] D. Holste, I. Grosse and H. Herzel, Phys. Rev. **E64**, 041917(2001).
- [11] D. Holste, I. Grosse, S. Beirer, P. Schieg and H. Herzel, Phys. Rev. **E67**, 061913(2003).
- [12] Y. Isohata and M. Hayashi, J. Phys. Soc. Jpn. **72**, 735(2003).
- [13] I. Grosse, P. Bernaola-Galvan, P. Carpena, R. RomJan-RoldJan, J. Oliver, H.E. Stanley, Phys. Rev. **E65** 041905(2002).
- [14] J.P. Lewis, T.E. Cheatham,III, E.B. Strikov, H. Wang and O.F. Sarkey, J. Phys. Chem. **B107**, 2581(2003).
- [15] D. Porath, G. Curiberti and R. Difelice, preprint "Charge Transport in DNA-based Devices" (2004).
- [16] L. Kari, Math. Intelligencer **19**, 9 (1997).
- [17] G. Paun, G. Rozenberg and A. Salomaa, *DNA Computing -New Computing Paradigms*, (Springer-Verlag, 1998)
- [18] D. Porath, A.Bezryadin, S. de Varies and C. Dekker, Nature (London) **403**, 635 (2000).
- [19] P. Tran, B. Alavi, and G. Gruner, Phys. Rev. Lett. **85**, 1564(2000).
- [20] J.X. Zhong, *Technical Proceedings of the 2003 Nanotechnology Conference and Trade Show*, vol.2, 105.
- [21] G. Cuniberti, L. Craco, D. Porath, and C. Dekker, Phys. Rev. B **65**, 241314(R) (2002).
- [22] K. Iguchi, Int. J. Mod. Phys. **B11**, 2405(1997).
- [23] K. Iguchi, J. Phys. Soc. Jpn. **70**, 593(2001).
- [24] Z. G. Yu and Xueyu Song, Phys. Rev. Lett. **86**, 6018(2001).
- [25] K. Iguchi, Int. J. Mod. Phys. **B17**, 2565(2003).
- [26] K. Iguchi, preprint " $\pi$ -electrons in a single strand of DNA: Revisited" (2003).
- [27] D. Hennig, Euro. Phys. J. B **30**, 211(2002).
- [28] D. Hennig, J.F.R. Archilla and J. Agarwal, Physica D **180**, 256(2003).
- [29] D. Hennig, E.B. Starikov, J.F.R. Archilla and F. Palmero, preprint "Charge transport in poly(dG)-poly(dC) and poly(dA)-poly(dT) DNA polymers", nlin.PS/0308003 (2003).
- [30] J. Ladik, Phys. Rep. **313**, 171(1999).

- [31] L. Shen, Y.-J. Ye and J. Ladik, Solid State Commun. **121**, 35(2002).
- [32] R. Bruinsma, G. Guner, M.R. D’Orsogna and J. Rudnick, Phys. Rev. Lett. **85**, 4393(2000).
- [33] E.I. Kats and V.V. Lebedev, JETP Letters **75**, 37(2002).
- [34] E.B. Starikov, J. Photochem. Photobiol. **C3**, 147(2002).
- [35] P. Damle, A.W. Ghosh and S. Datta, Chem. Phys. **281**, 171(2002).
- [36] A. Troisi and G. Orlandi, J. Phys. Chem. B **106**, 2093(2002).
- [37] A. Rodriguez *et al.*, Phys. Rev. Lett. **92**, 27404(2003).
- [38] H. Yamada, *Slow Dynamics 2003* (AIP Conference Proceedings, 2004), Ed. by M. Tokuyama and I. Oppenheim, in press.
- [39] J. Heinrichs, Phys. Rev. B **66**, 155434 (2002).
- [40] Y. Aizawa, C. Murakami and T. Kohyama, Prog. Theor. Phys. Suppl. **79**, 96(1984); Y. Aizawa, Chaos, Solitons and Fractals, **11**, 263(2000).
- [41] H. Yamada and T. Okabe, Phys. Rev. E **63**, 26203(2001).
- [42] A. Lahiri and L. Nilsson, Chem. Phys. Lett. **311**, 459(1999).
- [43] M. Milke, J. Phys. A: Math. Gen. **30**, L367(1997).
- [44] G.G. Kozlov, V.A. Malyshev, F. Domingues-Adame and A. Rodriguez, Phys. Rev. **B58**, 5367(1998).
- [45] F. Domingues-Adame, I. Gomez, A. Avakyan, D. Sedrakyan and A. Sedrakyan, Phys. Stat. Sol. (b) **221**, 633(2000).
- [46] P. Biswas, P. Cain, R.A. Romer, and M. Schreiber, Phys. Stat. Sol. (b) **218**, 205 (2000).
- [47] P.W. Brouwer, C. Mudry, B.D. Simons and A. Altland, Phys. Rev. Lett. **81**, 862(1998).
- [48] P.W. Brouwer, E. Racine, A. Furusaki, Y. Hatsugai, Y. Morita and C. Mudry, Phys. Rev. **B66**, 014204(2002).
- [49] F. Dyson, Phys. Rev. **B92**, 1331(1953).
- [50] B. Souillard, in *Chance and Matter* (North-Holland, Amsterdam 1986), Ed. by J. Souletie and J. Vannimenus and R. Stora.
- [51] L. Molinari, J. Phys. A: Math. Gen. **36**, 4081(2003), math-ph/0210042.
- [52] Y. Imry, Rev. Mod. Phys. **71**, S306(1999).
- [53] Y. Imry and J. Imry, *Introduction to Mesoscopic Physics 2nd edition*, (Oxford University Press, Oxford, 2002).
- [54] A. Tikhonov, R.D. Coalson and Y. Dahnovsky, J. Chem. Phys. **117**, 567(2002).

- [55] A. Tikhonov, R.D. Coalson and Y. Dahnovsky, J. Chem. Phys. **116**, 10909(2002).
- [56] J. Lehmann, S. Kohler, P. Hanggi, and A. Nitzan, Phys. Rev. Lett. **88**, 228305(2002).
- [57] K. Walczak, cond-mat/0308426.
- [58] H.-L. Wu and P.W. Phillips, Phys. Rev. Lett. **66**, 1366(1991).
- [59] H. Yamada, in preparation.
- [60] J. Ladik, *Quantum Theory of Polymers as Solids*, (Plenum Press, New York, 1988).
- [61] S. Roche, Phys. Rev. Lett. **91**, 108101(2003).
- [62] S. Roche, D. Biccout, E. Macia and E. Kats, preprint, "Long Rang Correlations in DNA: scaling properties and charge transfer efficiency" (2003).
- [63] W.P. Su, J.R. Schrieffer and A.J. Heeger, Phys.Rev. B**22**, 2099(1980).
- [64] K. Iguchi, RIKEN Review **6**, 49(1994).